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Accurate elastic and inelastic scattering factors from He to Ne using correlated wave functions

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X-ray elastic and inelastic scattering factors for He through Ne ground states are computed from configuration-interaction wave functions constructed from Slater-type orbitals. The formalism for computing these scattering quantities from multideterminantal wave functions and open-shell systems has been specifically addressed. The reliability of the present tabulations has been checked with the energies through sum rules. The effect of core, intershell, and valence electron correlations is analyzed.

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I. INTRODUCTION

X-ray [1] and high-energy electron scattering [2] have long been used to study electron correlation and chemical binding. With the advent of new x-ray [3] and high-energy electron scattering [4] techniques, more accurate information about electronic systems can be obtained. This demands high-quality theoretical data for comparison such as those for the atomic system Ne [4,5]. Accurate theoretical scattering factors are also required to facilitate the analysis of chemical binding for molecular systems. Due to the lack of highly correlated atomic scattering factors, earlier studies of chemical binding had to be carried out along with the correlation effect [6]. To directly extract the chemical binding effect from the experimental data, it is highly desirable to have both correlated elastic and inelastic scattering factors for atoms.

Electron correlation has long been recognized as an important factor for the accurate prediction of scattering quantities, especially the inelastic ones. For He, the computations [7–10] indicate a discrepancy of 6% in the inelastic scattering factors. Brown [11] found that for Li, the elastic scattering factors from restricted Hartree-Fock (HF) and correlated wave functions differ by 1–2% whereas the inelastic scattering factors can differ by as much as 10%. Peixoto *et al.* [12] studied the He and Ne atoms and found that for Ne, a 10% difference results from electron correlation. Both the elastic and inelastic scattering factors of Be have been calculated with correlated wave functions and similar observations of correlation effects on the scattering factors have been found [13,14]. A more comprehensive study on the scattering factors has been carried out by Tanaka and Sasaki [15]. Configuration interaction (CI) wave functions including only L-shell electron correlation were employed to compute the scattering factors from Be to Ne. These authors have concluded that even with only L-shell electron correlation considered, scattering factors, especially the inelastic ones, undergo changes of the order of 10% or more.

In this paper, the scattering factors for the ground states of He through Ne are calculated from CI wave functions and analyzed in terms of core, intershell, and valence electron correlations.

II. COMPUTATIONAL DETAILS

The elastic scattering factors, or atomic form factors, are the Fourier transformation of the electron charge density, the diagonal elements of the one-particle density matrix [16],

$$F(\boldsymbol{\mu}) = \int \rho(\mathbf{r}) \exp(i\boldsymbol{\mu}\cdot\mathbf{r})d\mathbf{r} = \int \gamma(\mathbf{r}|\mathbf{r}) \exp(i\boldsymbol{\mu}\cdot\mathbf{r})d\mathbf{r}\,, \quad (1)$$

where $\boldsymbol{\mu}$ is the momentum transfer variable. In Eq. (1), $\mu = 4\pi\sin(\theta)/\lambda$ and is given in atomic units (a_0^{-1}). Note that in the literature, other units (e.g., Å^{-1}) and/or variables [e.g., $\sin(\theta)/\lambda$] have also been used.

The total scattering intensity $I_t(\mu)$, which consists of elastic and inelastic components, is related to the Fourier transformation of the electron pair density, the diagonal elements of the two-particle density matrix [16],

$$I_t(\boldsymbol{\mu})/I_{\rm cl} = N + 2\int h(\mathbf{r}_{12}) \exp(i\boldsymbol{\mu}\cdot\mathbf{r}_{12})d\mathbf{r}_{12} = N + 2\int \Gamma^{(2)}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_1,\mathbf{r}_2) \exp(i\boldsymbol{\mu}\cdot\mathbf{r}_{12}) \times d\mathbf{r}_1 d\mathbf{r}_2\,, \quad (2)$$

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where N is the total number of electrons and $\gamma(\mathbf{r}_1|\mathbf{r}_1')$ and $\Gamma^{(2)}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_1',\mathbf{r}_2')$ are the one- and two-particle density matrices, respectively.

The inelastic scattering portion is easily found by subtracting the elastic one from the total, i.e.,

$$S(\boldsymbol{\mu}) = I_t(\boldsymbol{\mu})/I_{\text{cl}} - |F(\boldsymbol{\mu})|^2 \,. \tag{3}$$

Therefore, with known one- and two-particle density matrices, the calculation of elastic and inelastic scattering factors is straightforward. The construction of density matrices from wave functions have been outlined by Davidson [17] and a detailed account of the procedure can be found elsewhere [18]. Since the basic integrals for the computation of $F(\boldsymbol{\mu})$ and $S(\boldsymbol{\mu})$ from a single-Slater determinantal wave function have been described earlier [19], we will restrict our discussion to the complications that arise primarily from the multideterminantal nature of the CI wave functions used here.

The nonrelativistic CI wave function belonging to a set of L^2, S^2, L_z, S_z quantum numbers is written as

$$\Psi = \sum_{K}^{p} \Phi_K^p a_K^p \,, \tag{4}$$

where a_K^p are variational coefficients. Φ_K^p is the pth degenerate element of configuration K. It is obtained through successively orthonormalized L^2- and S^2-symmetric projections of Slater determinants $\{D_{K,\alpha}\}$ [20],

$$\begin{aligned}\Phi_K^p &= \mathcal{O}(L^2,S^2)\sum_{\alpha=1}^{p} D_{K,\alpha} b_{K,\alpha}^p \\ &= \sum_{\alpha=1}^{n_K} D_{K,\alpha} c_{K,\alpha}^p \,,\end{aligned} \tag{5}$$

where $\mathcal{O}(L^2,S^2)$ is the projection operator. It is clear that Φ_K^p is an expansion of a set of Slater determinants with appropriate coupling coefficients $c_{K,\alpha}^p$.

The orthonormal spin orbitals, which make up the Slater determinants $\{D_{K,\alpha}\}$ in Eq. (4), are further expanded into linear combinations of Slater-type orbitals (STO's),

$$\begin{aligned}\psi_i(\mathbf{r}) &= \sum_j c_{ji}\chi_j(\mathbf{r}) \\ \chi_j(\mathbf{r}) &= N_j R_j(r) Y_{l_i}^{m_i}(\theta_r,\phi_r) \\ R_j(r) &= r^{n_j-1}e^{-\zeta_j r} \,.\end{aligned} \tag{6}$$

The one- and two-particle density matrices, in terms of orthonormal spin orbitals, are written as

$$\gamma(\mathbf{r}_1|\mathbf{r}_1') = \sum_{j,k}\psi_j^*(\mathbf{r}_1)\psi_k(\mathbf{r}_1')\lambda_{jk} \tag{7}$$

$$\Gamma^2(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_1',\mathbf{r}_2') = \sum_{jkmn}\psi_j^*(\mathbf{r}_1)\psi_k(\mathbf{r}_1')\psi_m^*(\mathbf{r}_2)\psi_n(\mathbf{r}_2')\Lambda_{jkmn} \,. \tag{8}$$

The one-particle density matrix is generally block diagonalized according to the parity and m_l of the spin orbitals. For states with $L = 0$, the one-particle density matrix is further diagonalized into different l blocks. There is not much known about the symmetry properties of the two-particle density matrix. However, there are some simple rules governing all the nonzero two-particle density matrix elements. For example, the sum of the orbital angular momenta for particles $\mathbf{r}_1$ and $\mathbf{r}_2$ is equal to the sum of the counterparts for particles $\mathbf{r}_1'$ and $\mathbf{r}_2'$. Also, the sum of the magnetic momenta are constant for primed particles and unprimed particles.

The basic integral for elastic scattering is the Fourier transformation of a product of two spin orbitals,

$$f_{jk}(\boldsymbol{\mu}) = \int \psi_j^*(\mathbf{r})\psi_k(\mathbf{r})\exp(i\boldsymbol{\mu}\cdot\mathbf{r})d\mathbf{r} \,. \tag{9}$$

The spherically averaged elastic scattering factor then requires an integration over the angular dependence of $\boldsymbol{\mu}$,

$$\begin{aligned}f_{jk}(\mu) &= \langle f_{jk}(\boldsymbol{\mu})\rangle \\ &= \delta(l_j,l_k)\sum_q\sum_t N_q N_t c_{qj} c_{tk}\int R_q(r)R_t(r) \\ &\quad\times j_p(\mu r)r^2 dr \,,\end{aligned} \tag{10}$$

where $j_p(\mu r)$ is the pth order spherical Bessel function and $\langle\,\rangle$ indicates the spherically averaged quantity. Note the appearance of the δ function over orbital angular momenta in the above equation. This is to say that even though the one-particle density matrix is generally only diagonalized by parity, the contribution to the spherically averaged elastic scattering factors is from the l block-diagonalized ones. Other one-particle properties, such as the kinetic and nuclear potential energies, have the same feature. Therefore, we can write the elastic scattering factor from a multideterminantal wave function as

$$F(\mu) = \sum_{jk}\lambda_{jk} f_{jk}(\mu) \,. \tag{11}$$

For a single-determinant wave function, which is the case discussed in an earlier publication [19], one just needs to set $j = k$ and $\lambda_{jj} = 1$ or 0, depending upon whether the spin orbital is occupied or not, to recover the simple formula (18) in [19].

We have mentioned that the one-particle density matrix elements from the same parity but different l blocks do not contribute to the spherically averaged elastic scattering factors. Nevertheless, they have nonzero values for the total elastic scattering intensities $|F(\boldsymbol{\mu})|^2$, and this contribution has to be taken into consideration when we use Eq. (2) to find inelastic scattering factors. We notice that the differences between $\langle|F(\boldsymbol{\mu})|^2\rangle$ and $\langle F(\boldsymbol{\mu})\rangle^2$ are much smaller in atoms than in molecules [21].

To calculate the total scattering intensities, as given by Eq. (2), one needs basic integrals such as

$$\begin{aligned}f_{jk}f_{mn}^* = \int &\psi_j^*(\mathbf{r}_1)\psi_k(\mathbf{r}_1)\psi_m(\mathbf{r}_2)\psi_n^*(\mathbf{r}_2)\exp(i\boldsymbol{\mu}\cdot\mathbf{r}_{12}) \\ &\times d\mathbf{r}_1 d\mathbf{r}_2 \,,\end{aligned} \tag{12}$$

which, after spherical averaging, yields

$$\langle f_{jk}f^*_{mn}\rangle = \sum_p\sum_q\sum_t\sum_{q'}\sum_{t'}(2p+1)N_qN_tN_{q'}N_{t'}c_{qj}c_{tk}c_{q'm}c_{t'n}C^p(l_jm_j,l_km_k)C^p(l_nm_n,l_mm_m) \times \int R_q(r)R_t(r)j_p(\mu r)r^2dr \int R_{q'}(r)R_{t'}(r)j_p(\mu r)r^2dr\,, \qquad (13)$$

where the summation over p is restricted to $\max(|l_j - l_k|, |l_n - l_m|) \le p \le \min(|l_j + l_k|, |l_n + l_m|)$.

The obtained scattering quantities are connected with other atomic properties. This point has been discussed by Benesch and Smith [22] through the density matrix formalism. It can be shown that at small μ, the elastic scattering factor is approximated by

$$F(\mu) \sim N - \frac{\mu^2}{6}\langle r^2\rangle + \mathcal{O}(\mu^4)\,. \qquad (14)$$

Similarly, the small μ expansion of the total x-ray scattering intensity is

$$I_t(\mu)/I_{\rm cl} \sim N^2 - \frac{\mu^2}{3}\langle r_{12}^2\rangle + \mathcal{O}(\mu^4)\,. \qquad (15)$$

The calculated scattering quantities are also related to the energy contributions through sum rules. The one-electron contribution to the potential energy of the scatterer can be obtained [23] from elastic scattering factors,

$$\int_0^\infty F(\mu)d\mu = \frac{\pi}{2}\left\langle \frac{1}{r}\right\rangle, \qquad (16)$$

while the two-particle contributions can be obtained [24] from

$$\int_0^\infty \left[\frac{I_t(\mu)}{I_{cl}} - N\right] d\mu = \pi\left\langle \frac{1}{r_{12}}\right\rangle. \qquad (17)$$

Here atomic units for μ (a_o^{-1}) are assumed. The above two equations can be used to check the accuracy of the calculated scattering factors.

We start from the self-consistent-field (SCF) wave functions of Bunge *et al.* [25], which have $4s$ for He, $7s$ for Li and Be, and $7s5p$ for B to Ne. The above basis sets have then been expanded for the CI wave functions to $4s3p2d1f$ for He and $7s6p3d2f$ for the other elements. The STO exponents have been carefully energy optimized in a sequential order, and the entire process was repeated as many times as necessary to achieve energy convergence to within a fraction of a microhartree for the basis set considered [26]. All single and double substitutions have been included in the CI wave functions (SDCI) since these account for the major part of the electron correlation. The final CI energies with the designated basis sets are tabulated in Table I. The present results account for more than 80% of the total correlation energy (CE).

TABLE I. Total energies for He to Ne in the ground state (in a.u.). The SCF energy is from Ref. [25]. The total correlation energy is from Ref. [29].

Element	Energy SDCI	SCF	Fraction of CE recovered (%)
He	-2.90282	-2.86168	97.9[a]
Li	-7.47707	-7.43273	97.8
Be	-14.66046	-14.57302	92.7
B	-24.64244	-24.52906	90.8
C	-37.82935	-37.68862	90.0
N	-54.56960	-54.40093	89.6
O	-75.02044	-74.80940	81.8
F	-99.67474	-99.40935	81.8
Ne	-128.86165	-128.54710	80.6

[a] Reference [30].

III. RESULTS AND DISCUSSION

The elastic and inelastic scattering factors for He to Ne are tabulated in Tables II and III, respectively. The momentum transfer variable used in the tables is chosen to be $\sin(\theta)/\lambda$ with units of Å^{-1}. [Tables of $F(\mu)$ and $S(\mu)$ with other units are available from the authors.] The differences between the results from the present SDCI wave functions and the HF ones [19,27] are plotted in Figs. 1 and 2 for the elastic and inelastic scattering factors, respectively. Correlation effects on the total x-ray scattering intensity are displayed in Fig. 3.

For the elastic scattering factors, we found that the present data on He and Li agree well with the earlier tabulations [7,10,11]. For the other atoms, the present values differ slightly more from those of Tanaka and Sasaki [15] because of the inclusion of K- and intershell-electron correlation in the present work. The region that shows the largest discrepancy shifts gradually toward large μ as we move from Be to Ne. This may be related to the fact that the core electrons become more compact when the

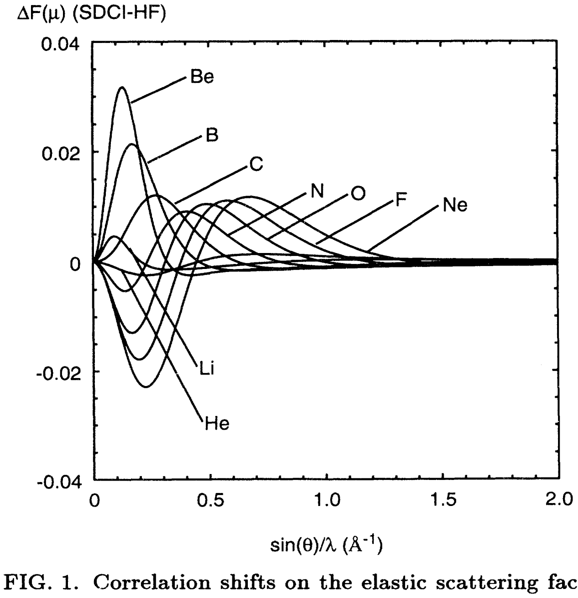

FIG. 1. Correlation shifts on the elastic scattering factors of He–Ne.

nuclear charge increases.

The inelastic scattering factors go through much larger changes under electron correlation. This is evident from a simple comparison of the corresponding curves from Fig. 1 and Fig. 2. At the correlated level, the inelastic scattering factors are, without exception, smaller than those predicted at the HF level. A closer look at Fig. 2 reveals that from Be to Ne, the negative peak gets deeper and the peak location shifts toward larger momentum transfer. The peak locations are 0.11, 0.15, 0.20, 0.25, 0.29, and 0.37 for elements Be to Ne, respectively. In addition, in the higher momentum transfer region, there is another peak resolved for Be to N. The locations are 0.74, 0.92, 1.09 and 1.26, respectively. This feature is also present in the total x-ray scattering plot (Fig. 3). We intend to relate the high momentum peak to the correlation from the core electrons. The following comparison seems to support such a linkage. This higher μ peak in Fig. 3 is completely missing from the study by Tanaka and Sasaki [15] (cf. Fig. 3) who have employed L-shell correlated wave functions. The peak they plotted (one for each element) appears at essentially the same location as the first peak displayed in this paper and has its origin in the L-shell correlation.

Also from Fig. 3, we notice that the Li curve has a positive peak in the small momentum transfer region. This peak has its origin in the intershell-electron correlation. For Li, the K-shell correlation results in a negative peak at the momentum transfer of 0.53. The location fits into the sequence of the second peak of the other elements. No L-shell correlation exists in Li. Thus, it is reasonable to associate the positive peak for Li to the

TABLE II. X-ray elastic scattering factors of He to Ne.

$\sin(\theta)/\lambda$ (Å^{-1})	He	Li	Be	B	C	N	O	F	Ne
0.00	2.0000	3.0000	4.0000	5.0000	6.0000	7.0000	8.0000	9.0000	10.000
0.01	1.9982	2.9865	3.9878	4.9886	5.9899	6.9910	7.9917	8.9923	9.9930
0.02	1.9930	2.9471	3.9518	4.9546	5.9597	6.9643	7.9667	8.9694	9.9719
0.03	1.9843	2.8848	3.8934	4.8990	5.9100	6.9201	7.9255	8.9315	9.9371
0.04	1.9722	2.8041	3.8147	4.8233	5.8418	6.8591	7.8684	8.8789	9.8887
0.05	1.9568	2.7103	3.7185	4.7294	5.7563	6.7821	7.7962	8.8121	9.8271
0.06	1.9383	2.6091	3.6082	4.6196	5.6551	6.6903	7.7096	8.7317	9.7527
0.07	1.9168	2.5056	3.4872	4.4966	5.5398	6.5846	7.6096	8.6386	9.6663
0.08	1.8925	2.4042	3.3590	4.3629	5.4124	6.4666	7.4973	8.5334	9.5683
0.09	1.8655	2.3081	3.2269	4.2214	5.2749	6.3376	7.3738	8.4172	9.4595
0.10	1.8362	2.2196	3.0940	4.0745	5.1292	6.1990	7.2403	8.2907	9.3407
0.11	1.8046	2.1397	2.9628	3.9247	4.9772	6.0524	7.0980	8.1552	9.2126
0.12	1.7710	2.0690	2.8357	3.7742	4.8209	5.8993	6.9482	8.0114	9.0761
0.13	1.7357	2.0070	2.7141	3.6249	4.6621	5.7411	6.7921	7.8606	8.9320
0.14	1.6989	1.9530	2.5995	3.4785	4.5022	5.5793	6.6310	7.7037	8.7812
0.15	1.6607	1.9061	2.4925	3.3364	4.3429	5.4150	6.4660	7.5417	8.6244
0.16	1.6215	1.8652	2.3936	3.1996	4.1853	5.2497	6.2982	7.3756	8.4627
0.17	1.5814	1.8292	2.3031	3.0689	4.0306	5.0843	6.1287	7.2064	8.2966
0.18	1.5407	1.7972	2.2207	2.9449	3.8797	4.9199	5.9583	7.0348	8.1272
0.19	1.4995	1.7683	2.1462	2.8281	3.7334	4.7574	5.7881	6.8618	7.9550
0.20	1.4580	1.7417	2.0792	2.7185	3.5923	4.5976	5.6187	6.6881	7.7809
0.22	1.3748	1.6931	1.9652	2.5213	3.3273	4.2886	5.2854	6.3414	7.4294
0.24	1.2924	1.6474	1.8743	2.3522	3.0869	3.9970	4.9632	5.9996	7.0776
0.25	1.2517	1.6250	1.8359	2.2776	2.9762	3.8587	4.8074	5.8319	6.9028
0.26	1.2116	1.6026	1.8015	2.2090	2.8718	3.7256	4.6555	5.6669	6.7295
0.28	1.1334	1.5574	1.7425	2.0888	2.6813	3.4756	4.3648	5.3461	6.3887
0.30	1.0582	1.5112	1.6937	1.9883	2.5142	3.2475	4.0925	5.0397	6.0577
0.32	0.9864	1.4640	1.6520	1.9045	2.3685	3.0411	3.8394	4.7490	5.7389
0.34	0.9184	1.4159	1.6151	1.8345	2.2421	2.8555	3.6056	4.4752	5.4336
0.35	0.8858	1.3916	1.5979	1.8038	2.1855	2.7701	3.4959	4.3447	5.2863
0.36	0.8543	1.3672	1.5813	1.7756	2.1329	2.6895	3.3909	4.2186	5.1429
0.38	0.7940	1.3181	1.5492	1.7255	2.0388	2.5416	3.1947	3.9793	4.8674
0.40	0.7376	1.2689	1.5179	1.6825	1.9576	2.4104	3.0159	3.7570	4.6076
0.42	0.6850	1.2200	1.4869	1.6448	1.8876	2.2943	2.8538	3.5513	4.3634
0.44	0.6361	1.1716	1.4558	1.6112	1.8269	2.1917	2.7070	3.3616	4.1346
0.45	0.6129	1.1476	1.4401	1.5956	1.7997	2.1450	2.6390	3.2725	4.0259
0.46	0.5906	1.1239	1.4244	1.5807	1.7742	2.1012	2.5745	3.1871	3.9209
0.48	0.5484	1.0771	1.3924	1.5523	1.7281	2.0212	2.4551	3.0268	3.7217
0.50	0.5094	1.0314	1.3601	1.5254	1.6875	1.9507	2.3476	2.8801	3.5366
0.55	0.4241	0.9226	1.2774	1.4617	1.6036	1.8077	2.1242	2.5662	3.1307
0.60	0.3540	0.8225	1.1935	1.3998	1.5362	1.7006	1.9531	2.3169	2.7973
0.65	0.2965	0.7316	1.1099	1.3373	1.4778	1.6178	1.8213	2.1196	2.5252
0.70	0.2494	0.6499	1.0282	1.2738	1.4239	1.5509	1.7186	1.9634	2.3040
0.80	0.1785	0.5121	0.8748	1.1453	1.3200	1.4433	1.5697	1.7392	1.9786
0.90	0.1300	0.4042	0.7385	1.0186	1.2161	1.3508	1.4631	1.5903	1.7617
1.00	0.0962	0.3203	0.6209	0.8986	1.1120	1.2622	1.3756	1.4829	1.6123
1.10	0.0723	0.2553	0.5212	0.7882	1.0097	1.1743	1.2959	1.3972	1.5032
1.20	0.0551	0.2048	0.4377	0.6888	0.9117	1.0870	1.2189	1.3222	1.4173
1.30	0.0426	0.1654	0.3681	0.6005	0.8196	1.0014	1.1430	1.2521	1.3444
1.40	0.0334	0.1346	0.3104	0.5231	0.7345	0.9189	1.0680	1.1843	1.2785
1.50	0.0265	0.1102	0.2625	0.4556	0.6567	0.8403	0.9946	1.1176	1.2161
1.60	0.0212	0.0909	0.2227	0.3971	0.5865	0.7664	0.9234	1.0521	1.1556
1.70	0.0172	0.0755	0.1897	0.3465	0.5233	0.6977	0.8551	0.9879	1.0964
1.80	0.0140	0.0631	0.1621	0.3029	0.4669	0.6342	0.7901	0.9255	1.0383
1.90	0.0116	0.0530	0.1391	0.2652	0.4167	0.5760	0.7288	0.8652	0.9814
2.00	0.0096	0.0449	0.1199	0.2327	0.3722	0.5228	0.6714	0.8074	0.9259
2.50	0.0042	0.0210	0.0601	0.1253	0.2150	0.3229	0.4414	0.5618	0.6777
3.00	0.0021	0.0109	0.0327	0.0716	0.1289	0.2032	0.2910	0.3872	0.4869
3.50	0.0012	0.0062	0.0191	0.0432	0.0806	0.1315	0.1950	0.2686	0.3490
4.00	0.0007	0.0037	0.0118	0.0274	0.0523	0.0877	0.1335	0.1888	0.2519
5.00	0.0003	0.0016	0.0052	0.0123	0.0244	0.0423	0.0669	0.0983	0.1362
6.00	0.0001	0.0008	0.0026	0.0063	0.0127	0.0225	0.0364	0.0547	0.0778

TABLE III. X-ray inelastic scattering factors of He to Ne.

$\sin(\theta)/\lambda$ (Å^{-1})	He	Li	Be	B	C	N	O	F	Ne
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.01	0.0033	0.0266	0.0188	0.0158	0.0133	0.0114	0.0104	0.0094	0.0084
0.02	0.0132	0.1025	0.0738	0.0626	0.0528	0.0453	0.0412	0.0372	0.0336
0.03	0.0296	0.2168	0.1617	0.1382	0.1171	0.1008	0.0919	0.0832	0.0752
0.04	0.0522	0.3545	0.2772	0.2396	0.2042	0.1765	0.1615	0.1463	0.1325
0.05	0.0807	0.5001	0.4139	0.3627	0.3116	0.2707	0.2484	0.2257	0.2047
0.06	0.1147	0.6405	0.5648	0.5031	0.4362	0.3811	0.3511	0.3199	0.2909
0.07	0.1538	0.7665	0.7233	0.6562	0.5748	0.5054	0.4677	0.4276	0.3898
0.08	0.1974	0.8737	0.8835	0.8179	0.7243	0.6412	0.5964	0.5472	0.5002
0.09	0.2451	0.9616	1.0405	0.9840	0.8815	0.7860	0.7351	0.6771	0.6209
0.10	0.2962	1.0322	1.1906	1.1513	1.0439	0.9377	0.8819	0.8157	0.7504
0.11	0.3502	1.0890	1.3312	1.3169	1.2089	1.0942	1.0351	0.9615	0.8875
0.12	0.4065	1.1357	1.4607	1.4787	1.3745	1.2536	1.1931	1.1130	1.0309
0.13	0.4646	1.1756	1.5785	1.6350	1.5390	1.4144	1.3542	1.2690	1.1794
0.14	0.5239	1.2116	1.6845	1.7844	1.7012	1.5753	1.5174	1.4282	1.3321
0.15	0.5840	1.2457	1.7792	1.9263	1.8600	1.7352	1.6814	1.5896	1.4877
0.16	0.6444	1.2791	1.8633	2.0600	2.0146	1.8934	1.8455	1.7523	1.6456
0.17	0.7046	1.3127	1.9378	2.1853	2.1645	2.0492	2.0088	1.9155	1.8050
0.18	0.7643	1.3469	2.0039	2.3022	2.3092	2.2021	2.1708	2.0787	1.9652
0.19	0.8231	1.3819	2.0625	2.4106	2.4484	2.3519	2.3309	2.2413	2.1257
0.20	0.8809	1.4177	2.1148	2.5108	2.5819	2.4982	2.4889	2.4029	2.2860
0.22	0.9921	1.4914	2.2045	2.6882	2.8313	2.7799	2.7973	2.7218	2.6049
0.24	1.0965	1.5670	2.2800	2.8377	3.0571	3.0462	3.0940	3.0335	2.9198
0.25	1.1459	1.6052	2.3141	2.9032	3.1612	3.1733	3.2377	3.1862	3.0753
0.26	1.1933	1.6434	2.3464	2.9632	3.2595	3.2964	3.3780	3.3366	3.2293
0.28	1.2819	1.7197	2.4076	3.0690	3.4394	3.5300	3.6483	3.6300	3.5324
0.30	1.3625	1.7952	2.4660	3.1589	3.5982	3.7468	3.9042	3.9129	3.8283
0.32	1.4353	1.8693	2.5228	3.2365	3.7377	3.9466	4.1450	4.1844	4.1164
0.34	1.5006	1.9414	2.5789	3.3045	3.8599	4.1296	4.3705	4.4438	4.3960
0.35	1.5305	1.9766	2.6069	3.3358	3.9151	4.2150	4.4774	4.5687	4.5323
0.36	1.5589	2.0113	2.6347	3.3655	3.9668	4.2963	4.5804	4.6904	4.6662
0.38	1.6107	2.0784	2.6901	3.4215	4.0606	4.4473	4.7749	4.9238	4.9265
0.40	1.6568	2.1427	2.7451	3.4737	4.1433	4.5837	4.9542	5.1435	5.1762
0.42	1.6975	2.2040	2.7996	3.5233	4.2168	4.7064	5.1189	5.3496	5.4149
0.44	1.7335	2.2620	2.8534	3.5712	4.2826	4.8166	5.2696	5.5421	5.6420
0.45	1.7498	2.2898	2.8800	3.5946	4.3131	4.8675	5.3400	5.6333	5.7512
0.46	1.7652	2.3168	2.9064	3.6177	4.3422	4.9157	5.4072	5.7211	5.8574
0.48	1.7932	2.3684	2.9583	3.6633	4.3969	5.0049	5.5325	5.8872	6.0610
0.50	1.8178	2.4167	3.0091	3.7082	4.4477	5.0853	5.6465	6.0408	6.2527
0.55	1.8670	2.5239	3.1301	3.8178	4.5623	5.2552	5.8882	6.3744	6.6817
0.60	1.9027	2.6131	3.2415	3.9236	4.6657	5.3925	6.0798	6.6451	7.0433
0.65	1.9286	2.6864	3.3425	4.0249	4.7627	5.5082	6.2342	6.8644	7.3451
0.70	1.9473	2.7463	3.4328	4.1210	4.8551	5.6100	6.3619	7.0430	7.5957
0.80	1.9709	2.8340	3.5825	4.2949	5.0286	5.7892	6.5667	7.3143	7.9772
0.90	1.9835	2.8910	3.6957	4.4421	5.1859	5.9490	6.7342	7.5146	8.2475
1.00	1.9905	2.9280	3.7794	4.5632	5.3253	6.0945	6.8821	7.6770	8.4501
1.10	1.9944	2.9519	3.8403	4.6605	5.4459	6.2260	7.0170	7.8183	8.6130
1.20	1.9966	2.9675	3.8843	4.7373	5.5483	6.3433	7.1407	7.9463	8.7526
1.30	1.9979	2.9778	3.9158	4.7972	5.6337	6.4463	7.2532	8.0640	8.8774
1.40	1.9987	2.9846	3.9385	4.8435	5.7040	6.5356	7.3545	8.1722	8.9915
1.50	1.9992	2.9892	3.9548	4.8792	5.7614	6.6120	7.4447	8.2712	9.0968
1.60	1.9994	2.9924	3.9666	4.9066	5.8079	6.6768	7.5242	8.3609	9.1937
1.70	1.9996	2.9946	3.9752	4.9275	5.8454	6.7314	7.5936	8.4416	9.2826
1.80	1.9998	2.9961	3.9814	4.9436	5.8755	6.7770	7.6537	8.5136	9.3637
1.90	1.9998	2.9971	3.9860	4.9560	5.8996	6.8150	7.7055	8.5774	9.4372
2.00	1.9999	2.9979	3.9893	4.9655	5.9190	6.8466	7.7498	8.6335	9.5033
2.50	2.0000	2.9995	3.9971	4.9892	5.9712	6.9390	7.8899	8.8233	9.7405
3.00	2.0000	2.9999	3.9991	4.9963	5.9890	6.9747	7.9506	8.9148	9.8663
3.50	2.0000	3.0000	3.9997	4.9986	5.9955	6.9889	7.9771	8.9581	9.9305
4.00	2.0000	3.0000	3.9999	4.9994	5.9981	6.9949	7.9889	8.9787	9.9632
5.00	2.0000	3.0000	4.0000	4.9999	5.9996	6.9988	7.9971	8.9940	9.9888
6.00	2.0000	3.0000	4.0000	5.0000	5.9999	6.9996	7.9991	8.9981	9.9962

TABLE IV. The nuclear potential (in a.u.) and electron-electron potentials (in a.u.) of He through Ne.

Element	V_{ne} (cal.)	V_{ne} [Eq. (16)][a]	V_{ee} (cal.)	V_{ee} [Eq. (17)][b]
He	-6.7525	-6.7525	0.94688	0.94688
Li	-17.1517	-17.1517	2.19871	2.19872
Be	-33.6983	-33.6983	4.38195	4.38192
B	-56.9673	-57.9672	7.68704	7.68705
C	-88.1939	-88.1936	12.5430	12.5430
N	-128.3786	-128.3778	19.2540	19.2540
O	-178.0890	-178.0874	28.0344	28.0345
F	-238.6615	-238.6586	39.2990	39.2990
Ne	-311.0874	-311.0823	53.3475	53.3476

Note: numerical integration by Simpson's rule.

[a] [0,500], 10000 points.

[b] [0,100], 2000 points.

TABLE V. The correlation effects on the nuclear potential (in a.u.) and electron-electron potentials (in a.u.).

Element	ΔV_{ne}(SDCI-HF)	$\Delta V_{ne}^{GB\mathrm{a}}$	ΔV_{ee}(SDCI-HF)	$\Delta V_{ee}^{GB\mathrm{a}}$
He	-0.0034	-0.0032	-0.0789	-0.0801
Li	-0.0053	-0.009	-0.0822	-0.08
Be	-0.0631	-0.074	-0.1072	-0.113
B	-0.0700	-0.07	-0.1521	-0.17
C	-0.0571	-0.07	-0.2166	-0.24
N	-0.0275	-0.05	-0.2953	-0.32
O	-0.0143	-0.01	-0.4215	-0.50
F	0.0058	0.04‡	-0.5495	-0.68[b]
Ne	0.0463	0.05	-0.6920	-0.82

[a] Ref. [28].

[b] 0.005 and -0.654, respectively, from Ref. [31].

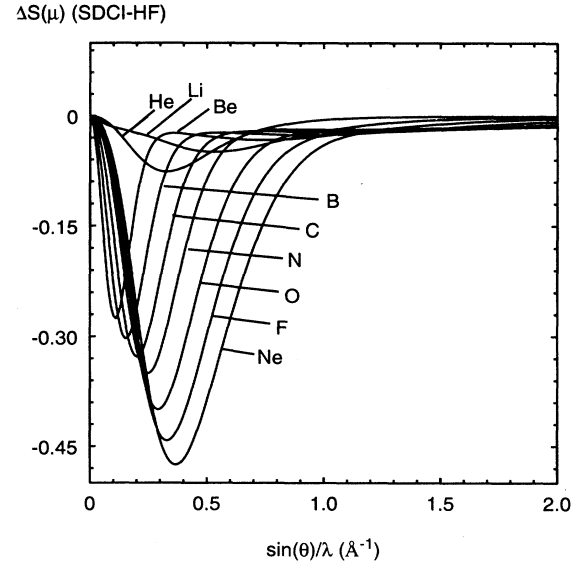

FIG. 2. Correlation shifts on the inelastic scattering factors of He–Ne.

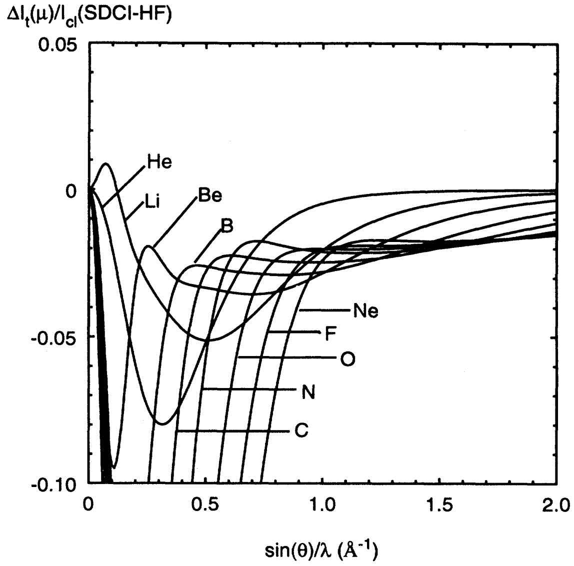

FIG. 3. Correlation shifts on the total x-ray scattering intensities of He–Ne.

intershell-electron correlation. This enhancement of intershell correlation in the total x-ray scattering intensity also shows up clearly in Be.

The change of the elastic scattering factors and the total x-ray scattering intensities at small μ allows us to extract useful physical properties. From Eq. (14), we conclude that a positive ΔF in Fig. 1 indicates $\langle r^2\rangle_{\rm corr} < \langle r^2\rangle_{\rm HF}$. This is the case for Li, Be, B, and C. The other elements, He, N, O, F, and Ne, have larger $\langle r^2\rangle$ at the correlated level. Similarly, from Eq. (15), it immediately follows that $\langle r_{12}^2\rangle$ becomes smaller for Li and larger for the other elements when electron correlation is taken into account.

We have checked the reliability of the present tabulation by invoking the sum rules given in Eqs. (16) and (17). Simpson's rule with equal spaced sampling points has been employed for the numerical integration. Due to a more rapid decay (as μ^{-8}) of the total x-ray scattering intensities [9], the integral converges to the true value with 2000 points ranging from 0 to $100a_0^{-1}$, shown in Table IV. However, the decay of the elastic scattering factors is much slower according to μ^{-4} [22] and in order to have good agreement with the true electron-nuclear potential, we have to use 10000 points up to $\mu = 500a_0^{-1}$. The results from Eq. 16 are still off for the heavier elements. Nevertheless, such examination should be able to verify that the scattering factors calculated from the CI wave functions are correct.

The correlation effects on the electron-nuclear (V_{en}) and electron-electron (V_{ee}) potential energies have also been investigated. The results are displayed in Table V. The trends are similar to those reported by Goruganthu and Bonham [28] based on a Z-expansion method with experimental total energies. The change of sign of ΔV_{ne} for F and Ne as predicted by Goruganthu and Bonham [28] is confirmed here. Except for the ΔV_{ne} of F, the quantitative agreement is also reasonably good [31].

The tabulated elastic and inelastic scattering factors can be compared directly with experiment for cases when incident photon energies are above the K-threshold of the target system. With other incident photon energies, modified scattering factors or other sophisticated theoretical models have to be used to account for the experiment. For more details on the applicability of elastic and inelastic scattering factors and different modification schemes, we suggest that readers consult a comprehensive review by Pratt [32] on elastic and a recent study by Bergstrom *et al.* [33] on inelastic x-ray scattering.

IV. CONCLUSIONS

Elastic and inelastic scattering factors for He through Ne have been predicted with highly correlated wave functions. The results are further compared with earlier correlated studies and checked through sum rules. The contributions from K-shell, L-shell, and intershell correlation to the scattering factors are analyzed. The energy components from the present scattering data compare favorably with those obtained by the Z-expansion technique.

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